

Using Satellite Data to Calibrate In-situ Temperature Measurements and to Improve their Assimilation into MODAS

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Abstract—The Modular Ocean Data Assimilation System (MODAS) creates temperature nowcasts in the world's oceans based on climatological models, in-situ measurements, and satellite observations. MODAS-Lite is a pared-down version that assimilates in-situ measurements to increase the accuracy of local nowcasts and gives the user control over the resolution of the nowcasts created. However, MODAS was created specifically for use in deep water, and care must be exercised in shallow, littoral waters. The present work shows how satellite data can be used to better control the data assimilation process in MODAS and to provide calibration for in-situ BT data sets.

I. INTRODUCTION

The Tactical Acoustic Measurement and Decision Aid project (TAMDA) is developing a new environmental sonobuoy that will directly measure ocean temperature and ambient noise, and indirectly measure bottom properties by inverting acoustic reverberation signals. In support of the TAMDA project, a sea test was conducted in early April 2003 in shallow water (about 90-130m deep) in the Gulf of Mexico near the Florida coast. The test involved a variety of environmental and acoustic measurements. Part of the project involves the development of assimilation and optimization algorithms to guide the selection of sonobuoy measurement locations in order to produce accurate temperature nowcasts using the Modular Ocean Data Assimilation System (MODAS).

The MODAS Adaptive Sampling Decision Aid (MASDA) is a research tool to determine optimal environmental sonobuoy placement under development by the Space and Naval Warfare Systems Command at the Naval Research Laboratory [1]. Its four methodologies are based on the hypothesis that the minimization of ocean temperature uncertainty tends to minimize error in temperature nowcasts created by MODAS. Sensor Placement for Optimum Temperature Sampling (SPOTS) is being developed by the Naval Air Systems Command at Neptune Sciences, Inc., as a near-optimal (but much faster) version of one of the MASDA methodologies. SPOTS also objectively performs a variety of assimilation tasks (such as bathythermograph (BT) quality control). The present work reports on recent findings with respect to BT assimilation into MODAS.

II. THE MODAS ASSIMILATION PROCESS

MODAS has two different forms, MODAS-Heavy and MODAS-Lite. MODAS-Heavy is used by the Naval Oceanographic Office to create daily nowcasts (so-called first-guess fields) over many ocean areas. MODAS-Lite is a general-release product that is used to a) create climatological fields from its internal climatology database, b) assimilate in-

situ data into first-guess and climatological fields, and c) interpolate any MODAS field to appropriate resolutions to suit the user's needs.

To assimilate in-situ data, MODAS (Heavy or Lite) uses an Optimal Interpolation (OI) algorithm to create both climatological and first-guess synthetic temperature profiles at required locations [2]. MODAS then performs several Quality Control (QC) tests. First, it creates synthetic climatological temperature profiles at all first-guess field locations and deletes any first-guess data that are not reasonably close to climatological expectations. If too many data points in any one profile are thrown out, the whole profile is thrown out. Then it creates synthetic climatological and first-guess temperature profiles at all BT locations, and applies the same QC criteria (once for each field) to determine which BT points and profiles to throw out. The surviving remainder of each BT profile is then smoothed vertically to fit a statistical model [3].

MODAS then uses the OI method to create its output field (at user-supplied latitudes, longitudes, and depths), relying on the altered first-guess field and the altered BTs wherever the first-guess field is dense enough, and relying on the climatological field and the altered BTs wherever it is not. The OI method weights all input data by their uncertainties and provides uncertainty estimates for the output, which is its primary advantage over other interpolation methods. Horizontal and vertical smoothing routines remove any large discontinuities to produce the final nowcast.

The OI method works by creating residual fields for each BT. Each first-guess synthetic profile point at the BT location is subtracted from the actual measurement there to determine the residue, which is then propagated outward as a Gaussian function of latitude, longitude, depth, and time (which means that older/distant BT data have less strength than identical newer/closer BT data). These residual fields are then added back into the gridded first guess field to create the final nowcast.

MODAS-Heavy uses this process to add recent in-situ measurements (if available to NAVOCEANO), but is mainly concerned with assimilation of satellite data (sea surface temperature and height). The surface temperatures are forced to agree (within measurement uncertainty limits) with the satellite data (which have been smoothed and QCed), and then steric height (actual sea surface height minus the expected tidal height) is used to compute the overall water densities at adjacent locations. The mixed-layer depths are then adjusted to create a synthetic temperature profile that agrees with these corrected densities.

In general, then, the MODAS assimilation process creates a symmetrical bulls-eye pattern around each measurement location. The shape is typically elliptical rather than circular

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because MODAS uses a parameter related to (and somewhat larger than) the Rossby radius of deformation (the scaling factor for the Coriolis effect) to determine the covariance scales to use in the Gaussian function. The Rossby radius both falls off and becomes more severely elliptical with increasing distance from the Equator. Use of the Rossby radius as a basis for the covariance scale appears well founded in the open ocean, but its validity in shallow areas, littoral waters, straits, and enclosed seas is unproven. Many researchers believe that other oceanographic processes predominate over the Coriolis effect in these areas. For this reason, MODAS allows a user to apply weighting factors to the E-W and N-S Rossby radii and to rotate the ellipse to align with land boundaries.

Figure 1 shows the first-guess field in the area where the TAMDA experiment was conducted (the star is the center of acoustic measurements) on the day (3 April 2003) when most of the acoustic measurements were conducted. No in-situ data are included in this nowcast. The color contours represent the water temperatures at 50m (left) and 0m (right). The shallow water to the north and east is much cooler than the water overlying the deeper ocean to the southwest. The gray areas represent regions shallower than the temperature field depth according to the bathymetry database used by MODAS. The black contour lines are bicubic splines fitted to the MODAS bathymetry data.

III. INTERPRETATION OF RESIDUAL FIELDS

If the first-guess temperature field has a complex structure, it can be difficult to gauge the effects of BT assimilations. In such cases, it is usually easier to interpret

the net residual field (which is the sum of the individual BT residual fields, but is computed as the difference of MODAS fields with and without BT assimilation). When only a few BTs are assimilated, or when they are widely spaced compared to the Rossby radius, interpretation of net residual fields is straightforward and obvious.

When multiple BTs are present and are closely spaced, however, there are reinforcement and interference effects which complicate the interpretation process. When the residuals have the same sign and a separation distance of less than one sigma (*i.e.*, distance/covariance distance), they reinforce each other and tend to merge into a net curve with a nearly Gaussian shape.

If closely spaced residuals are opposed in sign but nearly equal in absolute value, interference causes the net residual to be very weak, but it also causes the extrema of the net residual to behave counter-intuitively. Figure 2 shows two possibilities for two residuals of opposing sign, which are shown in blue. The negative Gaussian has 90% of the strength of the positive Gaussian. The red curve is the net (normalized) result, and the Xs are the maxima and minima for each curve. In the left panel, the individual residual centers are 0.2 sigmas apart, but the net residual extrema are 2.0 sigmas apart. In the right panel, the individual centers are farther apart (0.8 sigma), but the net extrema are closer together (1.8 sigmas). In both cases, the net residual is near zero in the vicinity of the residual centers. In two dimensions, the pattern for two interfering residuals is a dumb-bell (with lobes of opposing sign) aligned along the line connecting the BT locations, but the interference pattern can become much more complex when there are many BT locations.

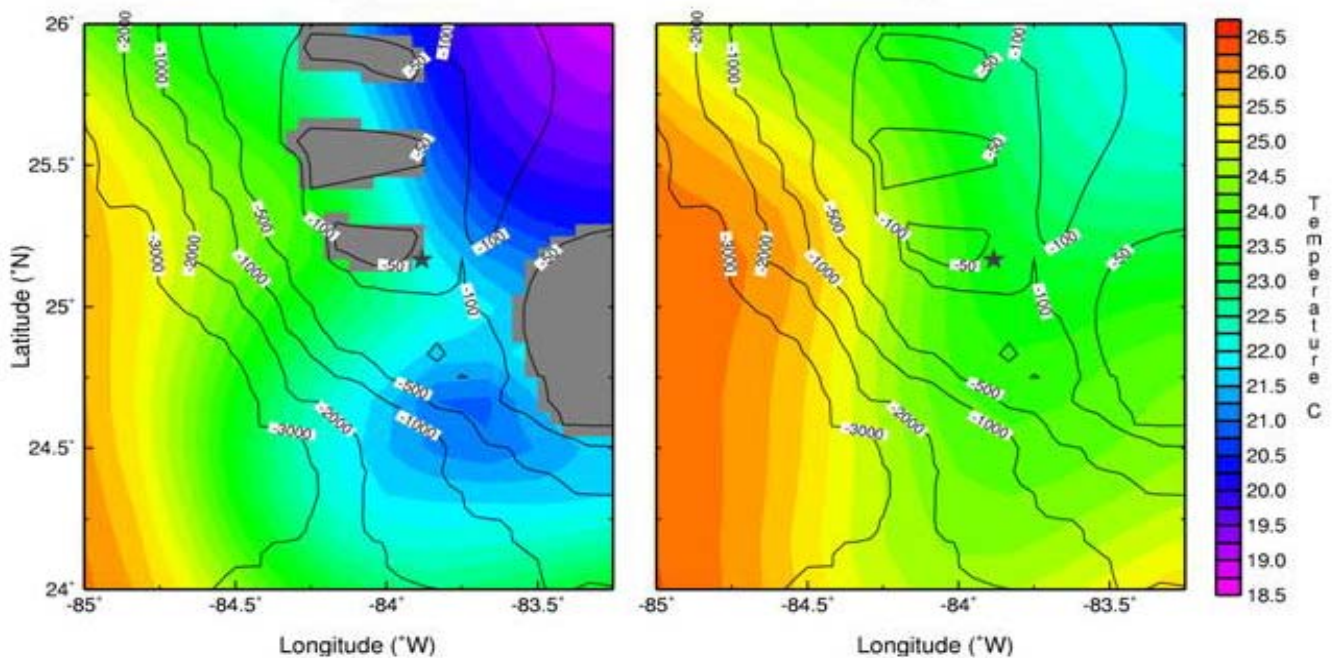


Figure 1. MODAS first-guess field in the experimental area on 3 April 2003 at 50m (left) and 0m (right). The star represents the center of the acoustic measurements.

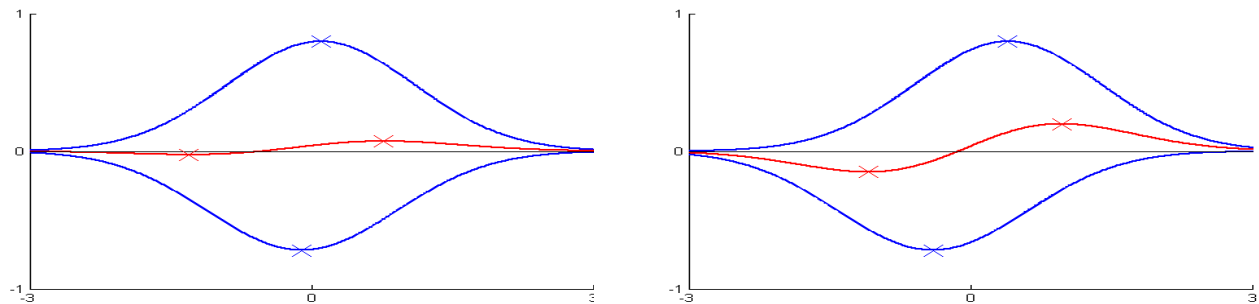


Figure 2. Demonstration of interference between Gaussian residuals. The vertical axis is temperature difference, the horizontal axis is separation distance normalized by the covariance distance (*i.e.*, sigmas). In the left panels, the separation is 0.2 sigma; in the right panels, 0.8 sigmas. In both cases, the negative residual is 90% as strong as the positive residual. The red curve is the net effect of the two residuals, and the Xs mark the local maxima and minima of each curve.

In the April test, the BT locations are scattered in two dimensions, and the spacings are very small compared to the Rossby radius at this latitude. Therefore, the type of pattern seen in net residual plots of MODAS fields can characterize the information added by the BTs. For instance, if the first-guess field were uniformly biased (compared to the ground truth, which in this case is the BTs), the net residual pattern would be a wide bulls-eye larger than the sampled area by about twice the covariance distance, but the sampled area itself would exhibit a fairly uniform and strong residue.

If instead the two fields (with and without BT assimilation) had the same mean value, but the east-west gradients of the two fields were different within the sampled area, then the net residual would be a large dumb-bell with negative and positive lobes, but the lobe separation would be fairly small. Large residues will be visible within the sampled area and will immediately begin to fall off at the edges of that area.

Zero-mean white noise tends to push the non-zero areas in the net residual out of the sampled area, so the lobes are more widely separated, and there may be many lobes of alternating sign. If the BT field has varying density and/or extent as a function of azimuth, there will likely be just two lobes centered along the line parallel to the direction with closest spacing or the fewest measurements. For a truly random drop pattern, however, the noise-generated lobes might be numerous and scattered randomly, but still outside the sampled area rather than within it.

In sum, then, when interpreting net residual plots for densely sampled areas, the salient features are: size, sign, strength, and number of the lobes, their location relative to the aggregate sampled area, and their locations relative to the individual sample locations. The relative strengths of bias and noise can be inferred by the degree of overlap between the sample area and the lobes.

IV. ASSIMILATIONS OF BT SETS

The first ten BTs were dropped from a boat on 2 April in a spiral pattern around the acoustic center of the test site with a spacing of roughly 1 nmi. On 3 April, the boat dropped an additional 5 BTs in the same area; meanwhile, twenty-four

BTs were dropped by air on a larger area, which extended from the initial BT area to the northeast. A storm had started at the end of March, and it persisted throughout the test. For simplicity, all assimilations into MODAS were performed using the 3 April NAVOCEANO first-guess field.

Figure 3 shows the MODAS nowcasts under normal (*i.e.*, default) assumptions for the vicinity of the study area after assimilating all BTs into the 3 April first-guess field (*cf.* Figure 1). The upper panels show color contours of temperature (in deg C). The lower panels show color contours of temperature residual (*i.e.*, difference) caused by the assimilation process, where shades of red represent increases in temperature and shades of blue represent decreases in temperature. The panels at left represent fields at 50m; at right, 0m. The average Rossby radius is about 50 km at the sea surface in deep water in this area [4]; the covariance scale used by MODAS is 130 km. However, such large covariance distances cannot be presumed to apply in such shallow water near the coast.

The residual plot at 0m has relatively simple lobes that cover only about half of the measurement locations, and their extrema are separated by about 3 sigmas (*i.e.*, multiples of the covariance distance). The wide separation of the extrema indicates either significant measurement noise or a very sharp (but real) temperature front at this depth. However, the simple shapes of the lobes indicate that few BTs differed from the first-guess field at 0m, which makes the noise interpretation more likely than the structural difference interpretation. We therefore looked for objective reasons to exclude some of the BTs.

The upper panel of Figure 4 shows the temperature profiles for all 39 BTs. The vertical axis is depth in meters, and the horizontal axis is temperature in deg C. The lower panel is a histogram of the profiles sorted into 5-m bins based on mixed layer thickness. The three which fall into the 3-8m bin are shown in red in the upper panel. Almost all BTs exhibit a large mixed layer, which is to be expected several days into a storm event with high winds. However, the profiles shown in red do not. The thickness of the mixed layer depends on the integral of wind-forced mixing over periods of 10-100 hours, so in the absence of shelter (such as an island), the mixed layer should have a relatively simple structure in the latter days of a storm event. Figure 5 shows

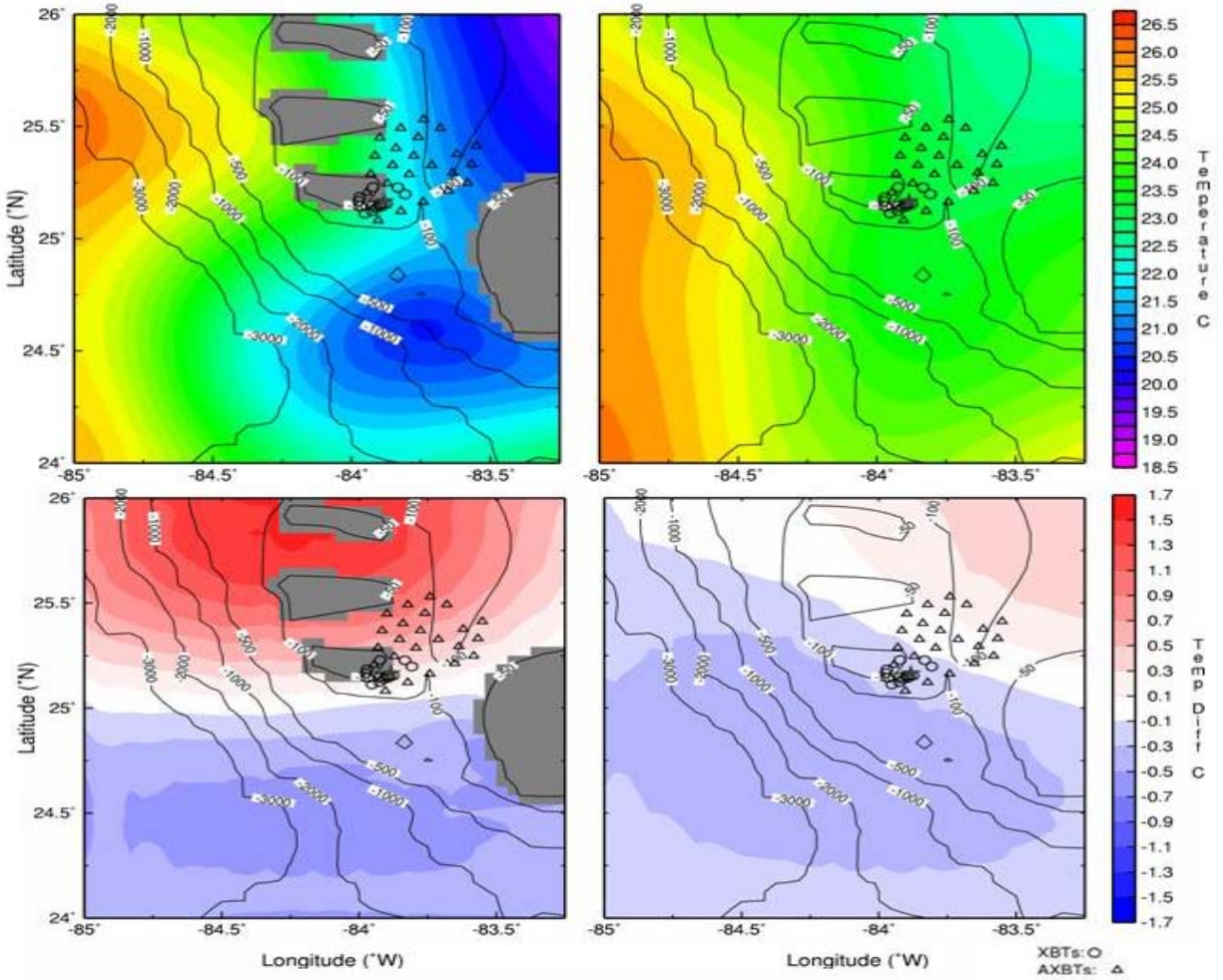
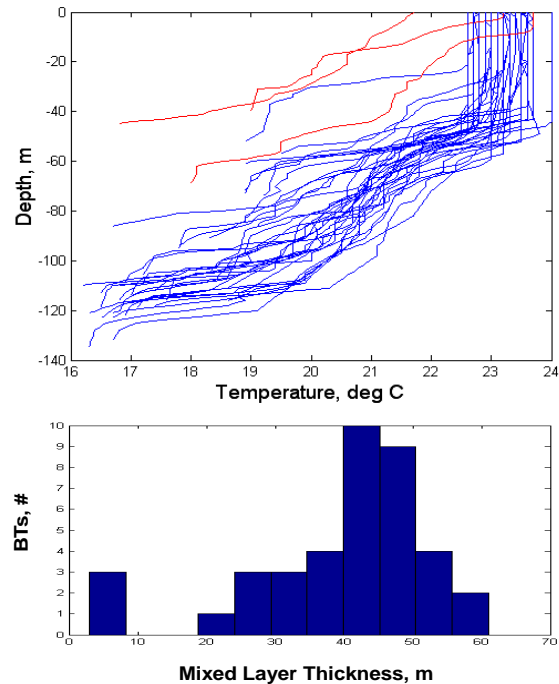


Figure 3. Nowcasts (upper panels) and residual plots (lower panels) for the study area on 3 April using all BTs and standard MODAS default assumptions. The panels at left correspond to 50m, at right to 0m. The boat-deployed BTs are represented as circles, the air-deployed BTs as triangles. Color contours represent temperature (upper panels) or temperature differences compared to the first-guess field (lower panels).

the mixed-layer thickness with (left panel) and without (right panel) the three apparent outliers earmarked in Figure 4. Removal of the apparent outliers significantly simplified the mixed layer, which increased our confidence that they should be removed from the dataset.

Figure 6 shows the revised residuals at 50m (left) and 0m (right) for the MODAS nowcasts with the outliers eliminated. The plotting conventions are identical to those used for the lower panels of Figure 3, which are the residuals without removal of the outliers. The positions of the extrema have shifted somewhat, but neither the separation nor the complexity have changed significantly. If noise were the cause of these residual patterns, the outliers were not the principal sources for that noise.

Figure 4 (to right). Temperature profiles for all BTs (upper panel), with depth in meters and temperature in deg C. Histogram of the thickness of the surface isothermal layer sorted into 5-m bins (lower panel). The red profiles in the upper panel correspond to the profiles that fell into the 3-8m bin in the lower panel.



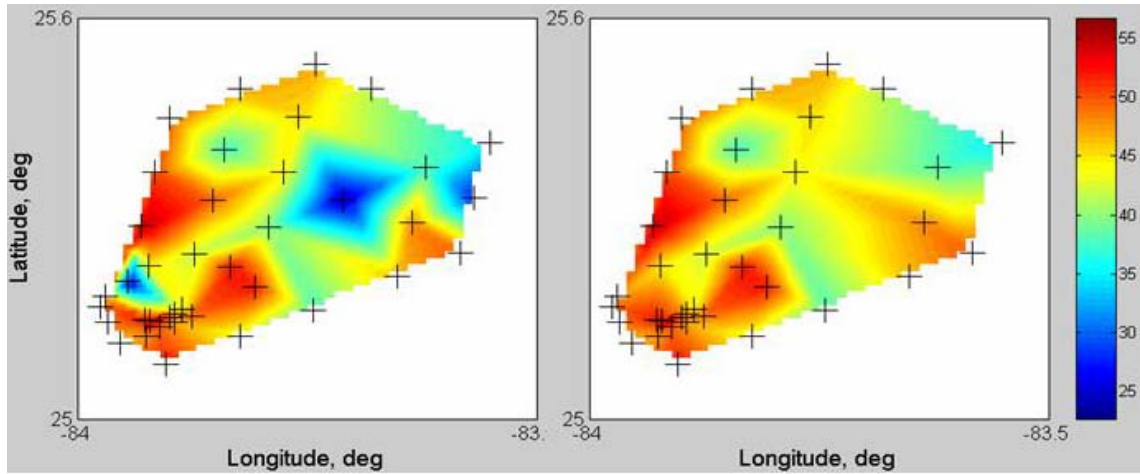


Figure 5. Surface isothermal (*i.e.*, mixed-layer) structure based on use of all BTs (left panel) and all BTs except the outliers (right panel). Color represents thickness of the layer in meters.

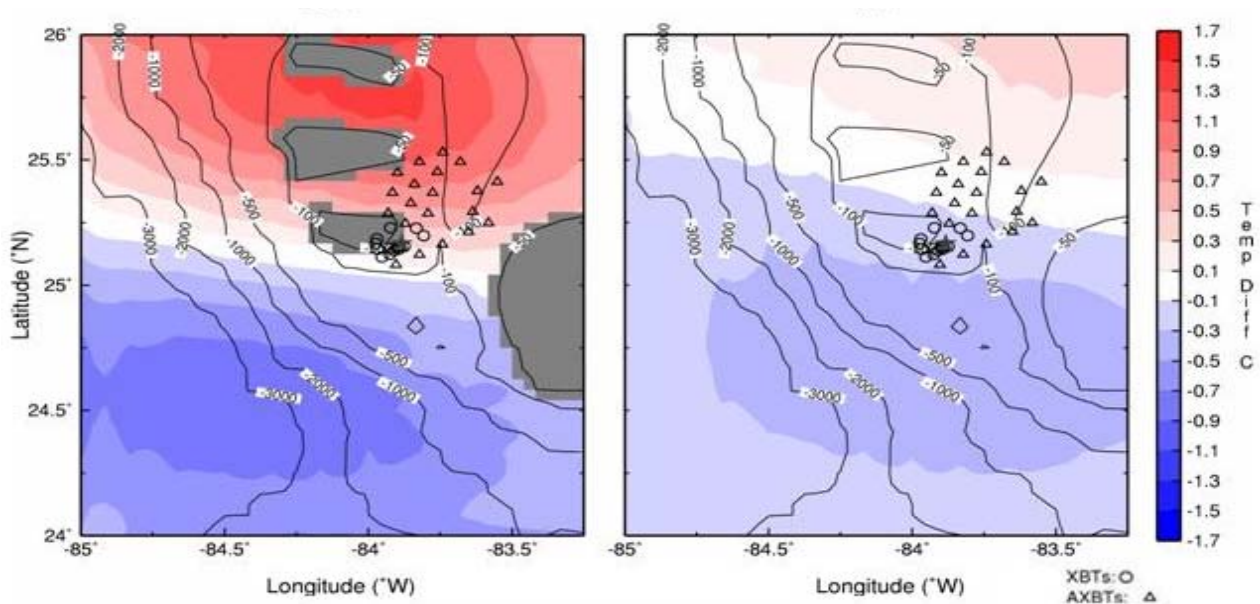


Figure 6. Residual plots for the study area on 3 April using all non-outlier BTs under standard MODAS default assumptions. The panel at left corresponds to 50m, at right to 0m. Color contours represent temperature differences compared to the first-guess field (Figure 1).

The Rossby radius default assumption for covariance distance in MODAS is generally suspect in shallow and littoral waters, yet the TAMDA system is designed primarily for use in just such waters. Covariance scale is generally presumed constant with depth, but increases at the surface due to mixed layer formation, so the surface covariance distance can be used as an upper bound for its mean value. Satellite observations of sea-surface temperature (MCSST) are usually available at the very high densities required for accurate covariance determination. These satellite data are recalibrated on very short time-scales and are generally very high in quality. However, due to cloud cover, some areas may be blank during any given time window.

The mean surface covariance distance was derived by binning the residual products for all satellite data point-pairs, taking the mean over each bin, and then using linear regression on all bins up to the first with a negative mean to determine the range (distance) at which the mean falls to $1/e$, or 0.3679. **Figure 7** shows the mean and standard deviation of all bins for the 3 April MCSST data. The mean surface covariance distance on 1 April was 7.65 km, on 2 April was 8.03 km, and on 3 April was 9.43 km, which are 5-7 times smaller than the Rossby radius expected at this latitude (50 km). The increase over time was expected, since wind-forced mixing tends to dominate surface covariance scales and the mixed layer depth tends to increase during a storm event.

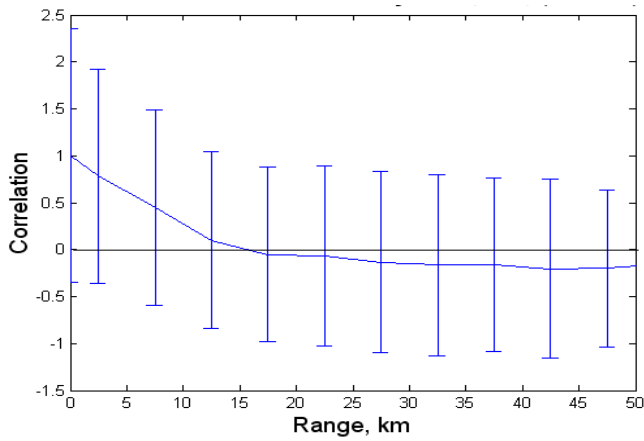


Figure 7. Covariance scale as a function of range within the study area, based on 478 NOAA-16 sea-surface temperature measurements for 3 April 2003. The e-folding distance is 9.4 km, compared to a Rossby radius of approximately 50 km.

The OI method was then used to estimate surface temperatures at all BT locations utilizing this covariance distance to provide a data source for calibration of the BTs. The mean and standard deviation of the calibration constants (ΔT s) were -0.36 ± 0.32 deg C for the BTs on 2 April and -0.45 ± 0.30 deg C for the BTs on 3 April. The ΔT s for the three outliers were not included in these statistics, but were respectively $+0.98$, -0.59 , and -1.14 deg C, or 1.3-2.5 standard deviations away from the mean.

Assuming that the manufacturing process is properly controlled, the calibration error for BTs is about ± 0.2 deg C and for BTs is about ± 0.15 deg C. Had the mean differences been zero, the increase in standard deviation could be possibly blamed on random handling damage, and the individual ΔT s could be taken as calibration errors (pure noise) without reservation. The biases (*i.e.*, the mean differences), however, require less likely hypotheses. That is, the ΔT s can only be presumed real if they make the nowcasts significantly more coherent. To test the hypothesis that the required correction was an offset, the ΔT for each profile was subtracted uniformly at all depths. Figure 8 compares the uncorrected profiles (top panel) to the corrected profiles (middle panel). The blue profiles are the 2 April BTs and the red profiles are the 3 April BTs (leaving out the 3 outliers). Correcting the profiles causes them to cluster strongly, and correctly shows the chilling trend at the surface expected during a storm. The bottom panel shows the standard deviation as a function of depth for the uncorrected profiles (dashed lines) and the corrected profiles (solid lines). The reduction of variance at the surface is very strong, but below the mixed layer there is no clear-cut trend.

A full-scale MODAS assimilation test of the corrected profiles was performed to corroborate whether the proposed corrections were realistic. Figure 9 shows the MODAS nowcasts and residual plots after assimilating the corrected (non-outlier) BTs. The plotting conventions are the same as used in Figure 3 and Figure 6. The assimilation also incorporates the satellite-derived covariance distance estimate (9.43 km). At 0m, the single residual lobe centered on the measurements implies that there is little or no noise in the

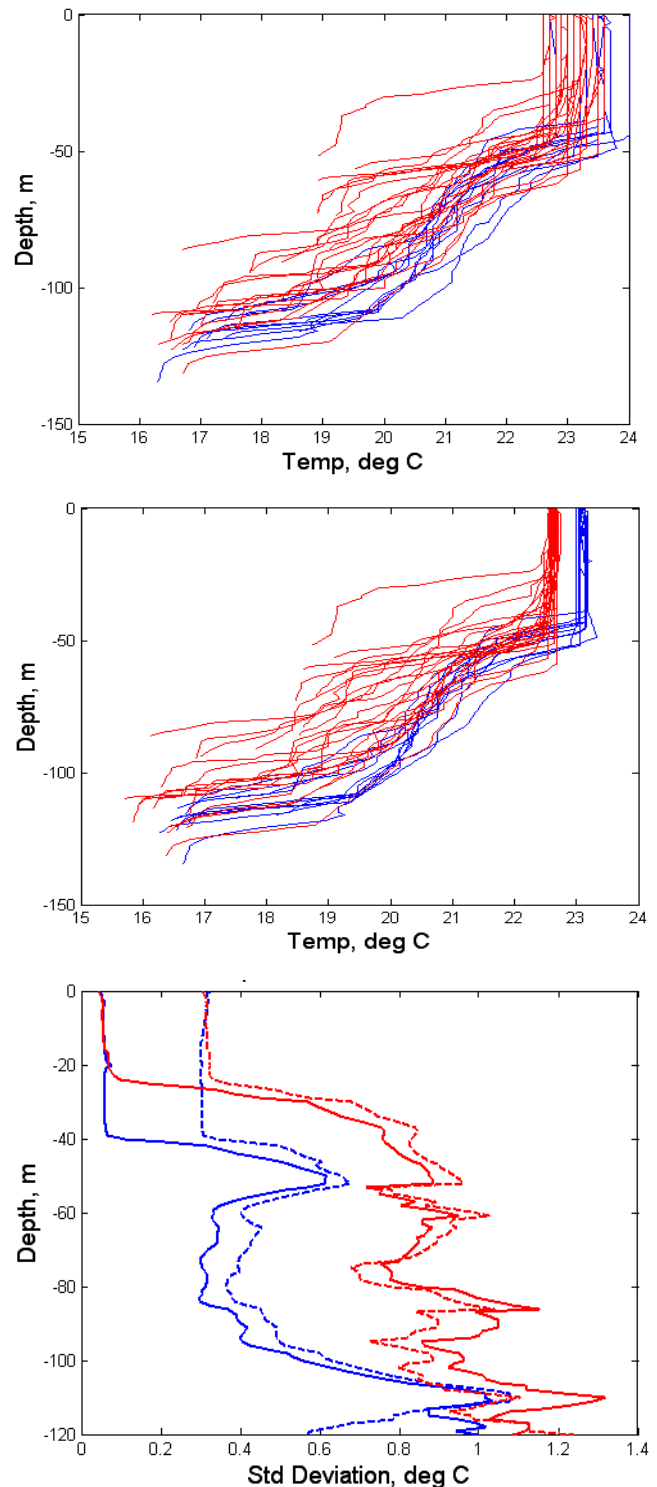


Figure 8. Uncorrected (top panel) and corrected (middle panel) BT temperature profiles, along with a comparison of their variances.

The vertical axis is depth in meters and the horizontal axis is temperature in deg C. In all panels, blue represents profiles on 2 April; red, 3 April. After adding the calibration corrections, the profiles cluster strongly based on date taken, as expected. In the bottom panel, dashed lines are the standard deviations as a function of depth for the uncorrected profiles; solid lines, for the corrected profiles.

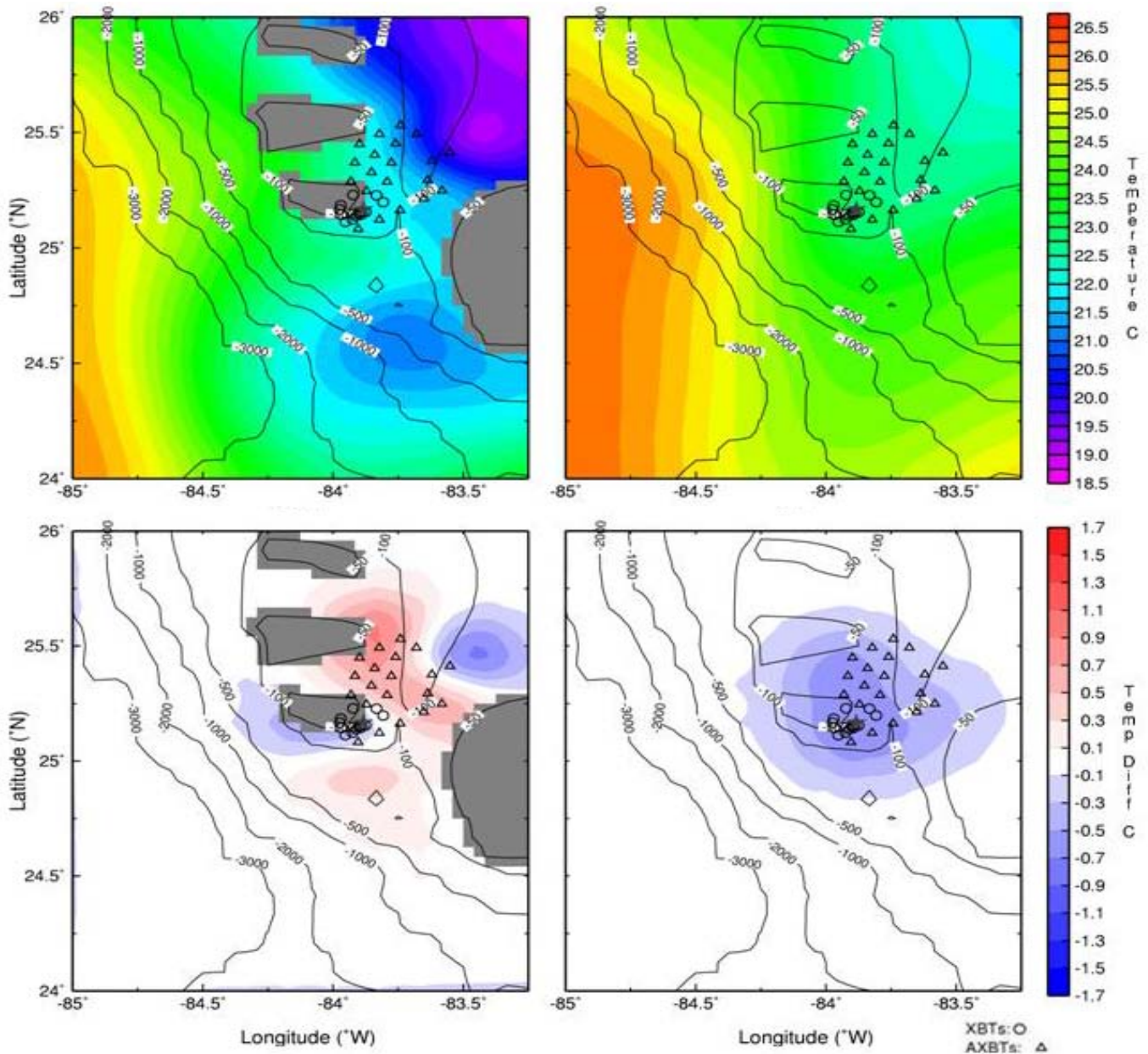


Figure 9. Nowcasts (upper panels) and residual plots (lower panels) for the study area on 3 April using corrected BT measurements, and incorporating the MCSST-derived covariance scale rather than the standard MODAS Rossby-radius assumption. The panels at left correspond to 50m, at right to 0m. Color contours represent temperature (upper panels) or temperature differences compared to the first-guess field (lower panels).

surface measurements, but the BTs have still added information to the nowcast. Since the measurements extend into the lesser-residual bands to the northeast, the bias uncovered by taking in-situ measurements can be presumed to fall off to zero in that direction, as shown. In all other directions, the area of highest bias is identical to the measurement area; the residuals taper off to zero because MODAS will only propagate the bias as dictated by the (small) covariance distance in those directions. In other words, it is possible that the 0.6 deg C cooling bias may extend a few more km, or even a few hundred more km to the southeast.

At 50m (left hand panel), there are now 4 lobes, but two are centered on the measurements, and therefore represent a real warming bias to the north and a cooling bias to the south at this depth. The other two lobes indicate that some noise is still present. Since the covariance scale is 5 times smaller, the diameters of these noise lobes are expected to shrink, but Figure 2 shows that their peaks will intensify by the same factor. Instead, they are slightly reduced in absolute terms (compared to using uncorrected profiles), and significantly reduced relative to expectation, which shows that the noise has in fact been significantly reduced.

I. CONCLUSIONS AND RECOMMENDATIONS

When BTs are dropped in unclouded areas, satellite data can be selected to provide synoptic information to calibrate those BTs. In cloudy weather, however, the situation is more complex. In principle, surface temperature calibration of BTs in deep water using nonsynoptic satellite measurements is roughly equivalent to surface temperature calibration of BTs using the first-guess MODAS field, since the first-guess field generally conforms to the satellite data. In practice, however, the turn-around time for MODAS-Heavy is such that more recent satellite observations are often available than those which have been incorporated into the most recent first-guess field available. In such cases, BT calibration using the satellite data is clearly preferable to BT calibration using the first-guess field.

However, in waters that are shallow, enclosed, or near land boundaries, the MODAS process may smooth the satellite data over unrealistically large areas. If nonsynoptic satellite data are first used to compute a more realistic covariance scale, and that scale is used to both estimate BT correction factors and control MODAS assimilation scales, the two surface temperature calibration processes are not equivalent. That is, recalibration using satellite data in these waters is superior to use of the first-guess field both in principle and in practice. In addition, the use of more realistic covariance scales in the MODAS assimilations of the BT data will provide more accurate subsurface nowcasts. Synoptic data, of course, are preferred for the BT correction steps whenever available.

These calibration factors are necessarily one-point corrections. When calibration is required over the whole water column, then other means must be used.

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